

Accurate determination of the superfluid-insulator transition in the one-dimensional Bose-Hubbard model

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Abstract. The quantum phase transition point between the insulator and the superfluid phase at unit filling factor of the infinite one-dimensional Bose-Hubbard model is numerically computed with a high accuracy. The method uses the infinite system version of the time evolving block decimation algorithm, here tested in a challenging case. We provide also the accurate estimate of the phase transition point at double occupancy.

Keywords: quantum phase transition, numerical methods

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INTRODUCTION

Ultra-cold atoms in optical lattices make possible detailed studies of basic condensed matter systems [1, 2, 3, 4]. While several applications have been envisaged ranging from high T_c superconductivity [5], disordered systems [6], spin models [7] or novel quantum magnets [8] - for a review, see [9] - the most basic model realized in such a setting is the Bose-Hubbard model (BHM) [10], which still defies an exact analytical description while exhibiting a nontrivial quantum phase transition [11] between a superfluid state and an insulator. Experiments, both three-dimensional [2] and one-dimensional (1D) [3], performed in additional confining atomic traps, led to realization of an inhomogeneous finite model. Still, from the theoretical perspective, the infinite system is the most challenging case. As in experiments, the typical numerical studies deal with finite size systems, with a possible extrapolation to infinite systems at the end. Such an extrapolation is always delicate, especially in the vicinity of the phase transition. Even simple quantities like the precise location of the phase transition point are still controversial, see below.

In the absence of an exact analytical result, one must rely on approximate results, such as the Bethe ansatz [12] or numerical studies, which are roughly of three different types: exact diagonalization for finite systems - limited to very small systems and thus unable to extrapolate to the infinite size -, Quantum Monte-Carlo (QMC) methods and Density Matrix Renormalization Group (DMRG) methods [13].

The Time Evolving Block Decimation (TEBD) algorithm [14, 15] is a novel variant of the DMRG method which can provide results for the temporal dynamics, but also for the eigenstates using imaginary time evolution. Recently, it has been extended to

1D lattice systems with nearest-neighbor interactions *of infinite size* [16, 17, 18]. It has been successfully tested on the integrable Ising model. It is yet to be seen whether really difficult problems can be attacked by this algorithm. The present work provides a partial answer to this question by addressing the challenging problem of the quantum phase transition of the BHM.

THE BOSE-HUBBARD PHASE TRANSITION

The Hamiltonian of the BHM, in dimensionless variables, reads

$$H = -J \sum_{r=1}^M (\hat{a}_{r+1}^\dagger \hat{a}_r + \text{h.c.}) + \frac{U}{2} \sum_{r=1}^M \hat{n}_r (\hat{n}_r - 1) - \mu \sum_{r=1}^M \hat{n}_r, \quad (1)$$

where M is the number of sites. We put it finite just for the introduction, as we shall consider $M = \infty$ for the actual calculation. \hat{a}_r^\dagger (\hat{a}_r) is the creation (annihilation) operator at site r , while $\hat{n}_r = \hat{a}_r^\dagger \hat{a}_r$. The total number of atoms $\hat{N} = \sum_{r=1}^M \hat{n}_r$ commutes with the Hamiltonian. In the thermodynamic limit of infinite systems, it is convenient to consider the particle density $\rho = \langle \hat{N}/M \rangle$ and the chemical potential μ .

Two parameters describe the model: the tunnelling rate J and the interaction strength U . Since physics of the BHM depends on the J/U ratio only, we set $U \equiv 1$ for convenience. The behaviour of the system as J/U is varied has been extensively discussed in a number of papers, see [10, 12, 19, 20, 21, 22, 23, 24, 26, 27, 28, 29, 30], thus we mention the most relevant details only. The Mott insulator phase occurs at integer occupation of sites for sufficiently small tunnelling. Within the Mott insulator regime, the density stays constant - the system is not compressible. Typically, at the phase boundary, the density changes and the superfluid regime is reached via a standard quantum phase transition. The interesting situation occurs when the phase transition is reached via a path of a constant integer density ρ . The model belongs then to the universality class of the XY model [10] and the phase transition is of the Kosterlitz-Thouless (KT) [31, 32] type.

In the present paper, we determine very accurately the J value at which the KT transition occurs for $\rho = 1$. This is a difficult task previously addressed using different methods yielding quite different results. The mean field theory [11, 33] yields $J_c \approx 0.086$. The Bethe ansatz allows for an analytical albeit approximate treatment [12] giving $J_c = 1/(2\sqrt{3}) \approx 0.289$. Early numerical values obtained via QMC [19] as well as renormalization group arguments [20] yielded a quite different value $J_c = 0.215$. Later numerical approaches came closer to the Bethe ansatz result. In particular, Kashurnikov et al. [21] found $J_c = 0.300 \pm 0.005$ in a QMC study while an exact diagonalization for $M = 12$ combined with renormalization group by the same group [22] yields $J_c = 0.304 \pm 0.002$. Other QMC approach [29] gave $J_c = 0.305 \pm 0.004$. Earlier diagonalization results [23] gave $J_c \approx 0.275 \pm 0.005$. High order perturbative expansion suggests $J_c = 0.26 \pm 0.01$ [24] in an excellent agreement with finite DMRG treatment [25] yielding essentially the same result. Yet other DMRG approaches gave interestingly different results. The periodic boundary conditions DMRG [26] gave $J_c \approx 0.298$ while the infinite size DMRG with periodic boundaries gave $J_c = 0.277 \pm 0.01$ [27]. The same

authors attempted a finite size DMRG with open boundary conditions (yielding a better convergence) giving $J_c = 0.297 \pm 0.01$ [28]. Therefore, the current algorithms disagree on the value of J_c . This is partially due to logarithmic finite-size effects close to the critical point of the KT transition [22, 28]. The accurate determination of J_c is thus an ideal testbed for algorithms dealing with infinite systems.

TIME-EVOLVING BLOCK DECIMATION ALGORITHM

The approach [16] used is an infinite variant of the TEBD algorithm [14, 15]. It belongs to a rapidly developing class of methods which utilise the understanding of quantum entanglement in complex systems to facilitate effective simulations of many-body quantum systems. All these methods have some links (see discussion in [34]) with the DMRG algorithms [13] extending them either to time evolution [14, 15] and to many dimensional systems [35, 36, 37]) A particularly interesting variant of the TEBD approach assumes translational invariance of the wavefunction and enables a treatment of explicitly infinite systems [16, 17, 18]. While we refer the reader to original papers for details, we sketch here the main idea.

The BHM Hamiltonian involves only nearest-neighbor interactions and can thus be written as a sum over consecutive sites r of reduced hamiltonians $h^{(r,r+1)}$. Each site is described by a Hilbert space of dimension D . We follow the imaginary time evolution, i.e., compute (we assume $\hbar = 1$ in the whole paper)

$$|\Psi(\tau)\rangle = \frac{\exp(-H\tau)|\Psi(0)\rangle}{\|\exp(-H\tau)|\Psi(0)\rangle\|}. \quad (2)$$

For large τ and a generic initial guess $|\Psi(0)\rangle$, such a procedure should yield a good approximation of the ground state provided there is a gap in the spectrum of the system.

We assume translational invariance of our system, i.e., $h^{(r,r+1)}$'s does not depend on site r . Moreover we restrict ourselves to wavefunctions that are invariant under shifts by one lattice spacing¹. The time evolution proceeds in the following way. The normalized wave function is Schmidt decomposed at site r as

$$|\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^{(r)} |\Phi_{\alpha}^{(\prec r)}\rangle \otimes |\Phi_{\alpha}^{(\succ r+1)}\rangle; \quad (3)$$

where χ is a finite Schmidt rank, the $|\Phi_{\alpha}\rangle$ states are an orthonormal set and $\sum_{\alpha} (\lambda_{\alpha}^r)^2 = 1$ for global normalization. As discussed in [14, 15], for low lying states, the λ_{α} values decrease rapidly, so that a good approximation of the state is obtained keeping only the few largest λ_{α}^r . The two consecutive left or right sub lattices states are related via tensors

¹ This assumption is not essential for the method and can be easily lifted, as pointed out in [16]. It excludes “charge density wave” or “checkerboard” solutions. Previous studies of the BHM indicate that the ground state is translationally invariant so there is no real limitation in the approach used.

$\Gamma^{(r)}$ as follows:

$$\begin{aligned} |\Phi_\alpha^{(\leftarrow r+1)}\rangle &= \sum_{\beta=1}^{\chi} \sum_{i=1}^D \lambda_\beta^{(r)} \Gamma_{i\beta\alpha}^{(r+1)} |\Phi_\beta^{(\leftarrow r)}\rangle |i^{(r+1)}\rangle, \\ |\Phi_\alpha^{(\rightarrow r)}\rangle &= \sum_{\beta=1}^{\chi} \sum_{i=1}^D \Gamma_{i\alpha\beta}^{(r+1)} \lambda_\beta^{(r+1)} |i^{(r)}\rangle |\Phi_\beta^{(\rightarrow r+1)}\rangle; \end{aligned} \quad (4)$$

where $|i^{(r)}\rangle$ is an orthonormal basis spanning the local Hilbert space at site r (e.g. the Fock basis for the BHM). In that way one obtains a so-called matrix product state (MPS) [38] representation of $|\Psi(\tau)\rangle$. The imaginary time evolution operation can be expressed as a product of elementary two-site evolution operators

$$U^{(r,r+1)} = \exp(-h^{(r,r+1)} \delta t), \quad \delta t \ll 1; \quad (5)$$

using the Suzuki-Trotter decomposition [39].

Now the crucial observation is that, for translationally invariant $|\Psi\rangle$, all $\Gamma^{(r)}$ and $\lambda^{(r)}$ are independent of r . The application of a two-site gate $U^{(r,r+1)}$ has two effects:

- it breaks for a moment the translational invariance (since sites r and $r+1$ are updated only);
- the resulting vector is not longer a MPS.

The latter is taken care of by a singular value decomposition of the resulting matrix and retaining only the χ largest eigenvalues (and corresponding vectors) - see [14, 15] for details and [16] for a graphical representation. This approximation brings the vector back into the MPS form. The modified $\Gamma^{(r)}$'s, $\lambda^{(r)}$'s are then updated for all the sites – the translational invariance is restored.

It is worth stressing that the repetition of this procedure allows one to act on two consecutive sites only, taking proper care of local updates of appropriate tensors. In the limit $\chi \rightarrow \infty$ and $\delta t \rightarrow 0$, the exact evolution is obtained. The error introduced by finiteness of δt is easily controlled (it varies as a power of δt depending on the order of the Suzuki-Trotter decomposition) while the strength of the method is that the number χ of not too small λ values remains reasonably small. As shown in [16], to facilitate convergence, one can take successively smaller and smaller time steps. In the following we use a simple second order Trotter expansion (which, according to our experience, seems to be the most efficient in imaginary time evolution when time steps are decreased).

APPLICATION TO THE BOSE-HUBBARD MODEL

To make the infinite-TEBD method work, additional parameters have to be adjusted. One of them is the maximal allowed occupation N_{max} at a given site (giving the dimension of the Hilbert space at each site, $D = N_{max} + 1$). In earlier DMRG calculations for mean unit occupancy typically $N_{max} = 4$ or $N_{max} = 6$ was used [25, 28]. We take $N_{max} = 6$, although the difference with $N_{max} = 4$ is small. The second important cutoff parameter

is the restriction on χ , the number of λ values retained at each step. This value can be quite small deep in the Mott insulator region, it has to be taken painfully large close to the KT transitions. This is costly since the execution time scales as χ^3 [16]. A satisfactory convergence of the correlation function

$$C(s) = \langle \hat{a}_{s+r}^\dagger \hat{a}_r \rangle \quad (6)$$

requires χ of the order of one hundred. Such correlation functions define the phase coherence of the condensate, we shall use them to determine the transition point.

In the Mott regime, the system has a finite gap, which implies that $|\Psi(\tau)\rangle$, eq. (2), converges exponentially fast at long times to the ground state, at a rate proportional to the energy gap. This is indeed what we numerically observe, with exponential convergence of the energy too. Thus, for a given time step we perform the imaginary time evolution until the slope of the energy curve w.r.t. imaginary time reaches a desired small threshold. Then the time step is decreased by a factor 2 and the procedure repeated until a computer accuracy limit for the time step is reached. While this procedure may not be optimal for speed, it assures the convergence of the results obtained.

It seems quite surprising that our results both for the energy and for the correlation function, Fig. 1, converge well even in the superfluid regime where the gap in the excitation spectrum should vanish. We indeed observe such a convergence, although apparently not fully exponential. We presently have no clear explanation of this behavior, which is under study. A plausible cause is the enforcement of translational invariance at each step of the algorithm. That restricts the spanned Hilbert space to the translationally invariant subspace killing, e.g., the possible excitations of low-frequency Bogolyubov modes in the superfluid regime. We carefully checked that all results presented in this paper are converged with respect to a modification of the (small) time step and an increase of χ .

The convergence of the long-range correlation functions is of particular importance. As discussed in [27, 28], at integer density, it should exhibit a power law $C(s) \propto s^{-K/2}$ for large s , on the superfluid side with K increasing up to $K = 0.5$ when the KT transition is approached. This is a behaviour typical for a Luttinger liquid characterising low energy excitations in the superfluid state. Fig. 2 reveals that it is indeed the case. As expected, the power law behaviour no longer holds on the Mott side of the transition. Here, deep in the Mott regime, an exponential decay of correlations is observed.

To estimate the KT transition point, a special case must be paid to keep a constant unit density. While for a finite system the particle number conservation can be explicitly used to keep the density fixed this is not the case for the infinite version of the code [16]. Instead, a chemical potential, μ , must be used and adjusted to keep a constant desired density. Our simulations were performed for different values of μ and the correlation functions shown (and used later to extract the transition point) were obtained for ρ well within $[0.999, 1.001]$ interval. To obtain slopes at $\rho = 1$ an appropriate interpolation of the results has been used. We observed that the power law coefficient in that interval changed weakly, the possible error in the transition point evaluation is included in the estimates given below.

The correlation functions $C(s)$ obtained at different J values are fitted with a power law on the superfluid side of the transition point. Since in the Mott regime the behaviour

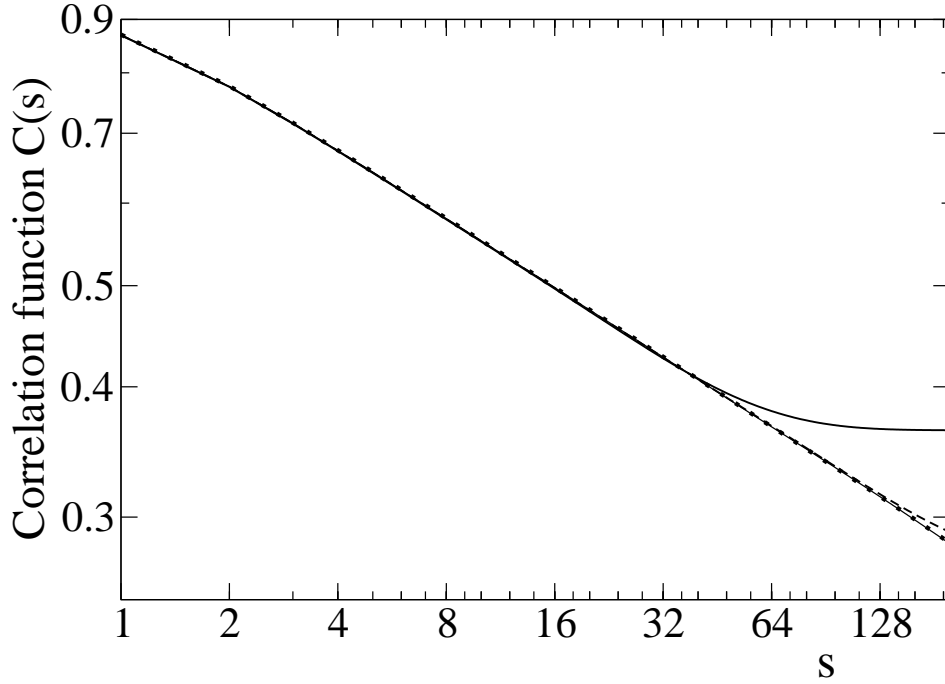


FIGURE 1. Correlation function $C(s)$ in the superfluid phase regime, $J = 0.32$. Solid line $\chi = 30$, dashed $\chi = 100$ while the dots and the underlying thin solid line correspond to $\chi = 150$ and $\chi = 200$, respectively. The last two sets almost coincide indicating the convergence with respect to χ . The linear behaviour in this log-log plot proves that the correlation function decays algebraically.

of the correlation function hardly resembles a power law (see Fig. 2), we make fits in different ranges of s exactly following the procedure of Kühner et al [28]. The obtained slopes (as a function of J) are interpolated to yield the transition point J_c . These points are collected in Table I for different s intervals. For comparison we reproduce also the results of [28]. While earlier DMRG results seem to be quite sensitive to the range of s values, our fits yield much closer and mutually consistent results. The comparison presented shows the power and accuracy of the infinite TEBD algorithm.

Clearly, fits for small s lead to misleading results, $C(s)$ for s below few tens (say 30) does not yet behave in the asymptotic power law way even in the superfluid regime. Given the accuracy of the method we can extend the evaluation of $C(s)$ to much larger s values, yielding global fits reported at the bottom of Table I. Note that those fits are in decent agreement with moderate s values of the order of 50.

We cannot, however, extend the calculation of $C(s)$ to much larger s values of the order of several thousands or more due to the numerical precision.

The KT transition point at unit density should be safely close to the value given by the last fit $J_c = 0.2975 \pm 0.0005$ where the (conservative) estimate of the error is coming from the comparison with other fits. While the obtained value is quite close to that

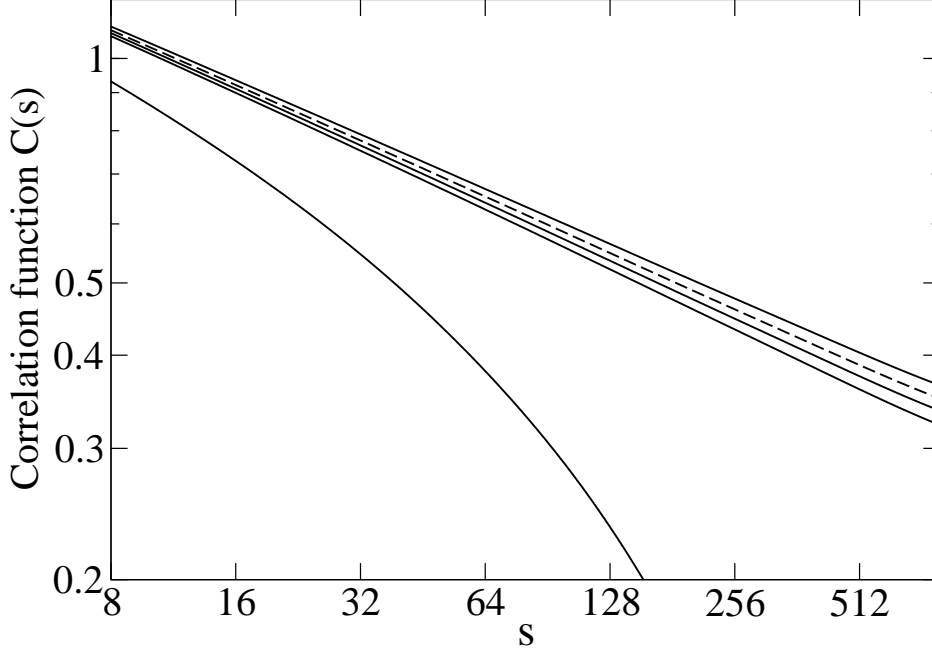


FIGURE 2. Correlation functions $C(s)$ for different values of J on a double logarithmic scale. From bottom to top: $J = 0.26, 0.29, 0.293, 0.296, 0.30$. The $J = 0.26$ curve in the deep Mott regime regime corresponds to a Mott insulator. As expected it resembles an exponential. In the deep superfluid regime, the power law is very well obeyed, that allows for accurate fits. Close to the transition, even on the Mott side, $C(s)$ shows transient behaviour for small s , then a region of an approximate power law behaviour, then for very large s an exponential tail is expected in the Mott regime. When approaching the critical point on the Mott side, this exponential region takes place at larger and larger s . In the range $s \leq 800$ shown in this plot, it is not visible expect for the lowest $J = 0.26$ curve. The $J = 0.296$ curve, the closest one to the critical curve $s^{-1/4}$, is shown by a dashed line.

reported previously [28], even our conservative error estimate makes the result more accurate by one order of magnitude.

Quite a similar approach can be used for a double occupancy case $\rho = 2$. Here, using the very same method, we obtain a benchmark value $J_c(2) = 0.175 \pm 0.002$. For that calculation the possible maximal occupancy of each site had to be larger or equal to 6. We have checked by a comparison of selected runs with those for even larger occupancy that the assumed maximal occupation is sufficient for the convergence.

CONCLUSIONS

To summarize, we have shown that the infinite TEBD algorithm [16] may be efficiently applied to nontrivial challenging problems such as the determination of the KT critical

TABLE 1. The location of the critical point J_c , estimated from different ranges of s value in the correlation function $C(s)$. The second column reproduces fits of [28], the third column yields present results.

s	J_c (DMRG)	J_c
$4 \leq s \leq 8$	0.2874 ± 0.0001	0.2868 ± 0.0006
$8 \leq s \leq 16$	0.2938 ± 0.0001	0.2933 ± 0.0002
$16 \leq s \leq 32$	0.2968 ± 0.0003	0.2955 ± 0.0001
$32 \leq s \leq 48$	0.3062 ± 0.0003	0.2970 ± 0.0001
$48 \leq s \leq 64$	0.3107 ± 0.01	0.2975 ± 0.0001
$100 \leq s \leq 250$		0.2980 ± 0.0001
$100 \leq s \leq 500$		0.2972 ± 0.0001
$50 \leq s \leq 500$		0.2975 ± 0.0001

point in the BHM. The accuracy is superior to that obtained by the standard DMRG approach. Surprisingly, converged results are also obtained in the superfluid regime. The restriction of the algorithm to the translationally invariant subspace, while justified for present ground state studies, may restrict the application of the method [16] to the real time evolution. There it could allow to treat “exactly” the dynamics of the quantum phase transition. Work in this direction is in progress.

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REFERENCES

1. D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
2. M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).
3. T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).
4. D. Jaksch and P. Zoller, Ann. Phys. (N.Y.) **315**, 52 (2005).
5. W. Hofstadter *et al.*, Phys. Rev. Lett. **89**, 220407 (2002).
6. A. Sanpera *et al.*, Phys. Rev. Lett. **93**, 040401 (2004).
7. L.M. Duan, E. Demler, and M.D. Lukin, Phys. Rev. Lett. **91**, 090402 (2003).
8. B. Damski *et al.*, Phys. Rev. Lett. **95**, 060403 (2005).
9. M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
10. M.P.A. Fisher, P.B. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B **40**, 546 (1989).
11. S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge UK, 2001).
12. W. Krauth, Phys. Rev. B **44**, 9772 (1991).
13. S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
14. G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).
15. G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004).
16. G. Vidal, Phys. Rev. Lett. **98**, 070201 (2007).

17. R. Orus and G. Vidal, <http://arxiv.org/abs/0711.3960v2>
18. I. P. Mc Culloch, <http://arxiv.org/abs/0804.2509v1>
19. G. G. Batrouni and R. T. Scalettar, Phys. Rev. B **46**, 9051 (1992).
20. K. G. Singh and D. S. Rokhsar, Phys. Rev. B **46**, 3002 (1992).
21. V. A. Kashurnikov, A. V. Krasavin, and B. V. Svistunov, Pis'ma Zh. Eksp. Teor. Fiz. **64**, 92 (1996) [JETP Lett. **64**, 99 (1996)].
22. V. A. Kashurnikov and B. V. Svistunov, Phys. Rev. B **53**, 11776 (1996).
23. V. F. Elesin, V. A. Kashurnikov, and L. A. Openov, Pis'ma Zh. Eksp. Teor. Fiz. **60**, 174 (1994) [JETP Lett. **60**, 177 (1994)]. 11 776 (1996).
24. N. Elstner and H. Monien, Phys. Rev. B **59**, 12184 (1999); cond-mat/9905367 (unpublished).
25. S. Rapsch, U. Schollwöck, and W. Zwerger, Europhys. Lett. **46**, 559 (1999).
26. R.V. Pai, R. Pandit, H.R. Krishnamurthy, and S. Ramasesha, Phys. Rev. Lett. **76**, 2937 (1996).
27. T.D. Kühner and H. Monien, Phys. Rev. B **58**, R14741 (1998)
28. T.D. Kühner, S.R. White, and H. Monien, Phys. Rev. B **61**, 12474 (2000).
29. L. Pollet, PhD Thesis, Universiteit Gent 2005, <http://www.nustruct.ugent.be/doc/thesislode.pdf>.
30. B. Damski and J. Zakrzewski, Phys. Rev. A **74**, 043609 (2006).
31. J. M. Kosterlitz nad D. J. Thouless, J. Phys. C **6**, 1181 (1973).
32. F. D. M. Haldane, Phys. Rev. Lett. **47**, 1840 (1981).
33. W. Zwerger, J. Opt. B: Quantum Semiclass. Opt. **5**, S9 (2003).
34. A.J. Daley *et al.*, J. Stat. Mech.: Theor. Exp. P04005 (2004).
35. F. Verstraete and J. I. Cirac, cond-mat/0407066 (unpublished); F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
36. L. Cincio, J. Dziarmaga, and M.R. Rams, Phys. Rev. Lett. **100**, 240603 (2008).
37. J. Jordan *et al*, <http://arxiv.org/abs/cond-mat/0703788v3>
38. M. Fannas, B. Nachtergaele and R. F. Werner, Comm. Math. Phys. **144** 443 (1992); S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).
39. M. Suzuki, Phys. Lett. A **146**, 319 (1990).